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NUMERICAL CALCULATIONS OF BLAST WAVES[*]

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SUMMARY

In the theory of blast waves, extensive numerical calculations have become a standard tool. As exemplified by the collaborative work of Boyer, Brode, Glass and Hall (1958), such solutions can provide valuable interpretation for experimental programs. Conversely, the application of such theoretical solutions to laboratory or field experience provides a desirable check on the limitations and physical approximations of the theory. These factors have prompted the present paper, in which the general steps in proceeding from physical assumptions to numerical answers are outlined for solutions by a Lagrangean coordinate, artificial viscosity method.

CONTENTS

I. INTRODUCTION

During the past two decades there has been an increasing ability as well as a continuing interest in describing the hydrodynamic consequences of explosions. The history of shock hydrodynamics from explosive sources and the motivations for investigations in this field make an interesting subject for discussion, but for the purposes of this paper attention will be restricted to those developments which have led to the current ability to carry out numerical computations describing in detail the hydrodynamic parameters associated with explosions.

After the fundamental physics governing the thermodynamics and hydrodynamics of explosions became evident, a number of investigators were successful in formulating analytical approximations for explosion phenomena. One type of solution, which has been variously expressed and derived, is useful in describing the early phases of an intense explosion. This solution, is of a similarity nature, i.e. one in which space and time are simply related and in a manner which allows the partial differential equations of motion to be reduced to ordinary differential equations. It is valid for the strong shock regime of point source explosions in an ideal gas. The most widely known version is that of G. I. Taylor,[1] however, both Sedov[2] in Russia and von Neumann[3] in the United States, at about the same time and independently, arrived at comparable solutions. These were all accomplished during World War II. Aside from some quite different treatments of other aspects of explosions this strong shock, point source, ideal gas solution stood without significant improvement for many years as the best description of the early phases of intense explosions. The Kirkwood-Brinkley similarity solution,[4] invented to describe high

explosive blasts also originated during World War II as did a weak shock, no similarity semiacoustical treatment by Bethe.[3] None of these solutions, however, was of sufficient generality to meet the growing requirements for complete specification of blast parameters, since in each case the form of the solution was forced by the similarity assumption or (as in the case of Bethe's solution) the limiting physical assumptions.

Similarity solutions, which serve to reduce the equations of motion to ordinary differential equations, were not possible outside of the strong shock regime except for very special circumstances. von Neumann was among the first to recognize the necessity of resorting to numerical methods for the more general solutions of the blast wave problems. Being also a pioneer in the development of high speed electronic computers, he foresaw the usefulness of such machines in performing truly prodigious numerical calculations. His continued interest in both machines and blast wave problems was instrumental to the development of a number of powerful techniques. In any methods of solution, special treatment of shock wave propagation is required. One early technique was to fit separately the shock position by means of the governing conservation laws across the shock front, and then calculating separately the effects of the adiabatic expansion behind the shock.[5] To the same end von Neumann and Richtmyer introduced artificial viscosity,[6] the effect of which was to spread shock discontinuities in such a way that they could be treated in a general scheme.[7] Later a partially successful method was developed by Lax which accomplished the same spreading without the introduction of special viscous terms.[8] Numerous early attempts at numerical computations proved successful. Notable among these were

calculations by von Neumann and Goldstein,[5] by Wecken[9] and by the present author.[7] One strong impetus for the development of methods of computing general hydrodynamic shock problems was in the development of nuclear weapons, and much of the pioneer work in such methods originated in the Los Alamos Laboratory of the AEC. Considerable interest in the effects of weapons, both nuclear and high explosive, prompted further development in other laboratories and institutions. Attention will be focused in the following section on one such method of approaching numerical calculations of hydrodynamic motions in compressible fluids.

The intent is not to provide the audience with an ability to program and run shock problems, since such an objective should require a more ambitious course and would lead through details of the flow diagraming of the program logic and bookkeeping methods. A portion of that sort of detail may be found in Refs. 10 and 11. Rather, the object here is to acquaint those interested in the nature of numerical methods with one such method in sufficient detail to allow them a fair evaluation of the effort and/or ease of formulating such techniques and of using such a scheme to solve a number of interesting problems.

II. A METHOD OF NUMERICAL CALCULATION

The problem presented by explosions lies in the solution of a set of nonlinear, partial differential equations representing the conservation of mass, momentum and energy. These conservation laws may be expressed mathematically in several ways, but are generally formulated in terms of either Eulerian or Lagrangean coordinates. The Eulerian form is an expression of the conservation laws as viewed from coordinate systems fixed in space and the Lagrangean form is an expression of the same conservations in terms of a fixed set of masses or gas particles, so that a solution in the Eulerian case represents the history of the blast wave at a fixed point while in the Lagrangean system a solution describes the experience of a particle (or a volume of gas) as it moves about. The set of equations below is one representation of these conservation laws in a Lagrangean system for a spherically symmetric explosion. In these equations the Lagrangean variable or mass coordinate is characterized by the mass per steradian, i.e., $m = \rho_1 R_o^3/3$ where ρ_1 is the initial density of the gas and R_o is its initial position.

$$\frac{1}{\rho} = V = \frac{1}{3} \frac{\partial R^3}{\partial m} \ , \qquad \text{conservation of mass;} \qquad (1)$$

$$\frac{\partial u}{\partial t} = - R^2 \frac{\partial}{\partial m} (P + Q) \ , \qquad \text{conservation of momentum;} \qquad (2)$$

$$\frac{\partial E}{\partial t} = - (P + Q) \frac{\partial V}{\partial t} + D \ , \qquad \text{conservation of energy;} \qquad (3)$$

$$\left. \begin{array}{l} E = E(T,V), \ P = P(T,V) \\[2mm] \text{or} \\[2mm] P = P(E,V), \ T = T(E,V) \end{array} \right\} \ , \ \text{equations of state;} \qquad (4)$$

$$u = \frac{\partial R}{\partial t} \, , \qquad\qquad \text{particle velocity.} \qquad\qquad (5)$$

In these equations the symbols are defined as follows:

V - specific volume

R - radial distance

u - particle velocity

P - pressure

Q - artificial viscosity pressure

E - specific internal energy

T - temperature

D - specific energy loss (or source) rate

m - mass/steradian

t - time

In solving these equations for a specific set of initial and boundary conditions by numerical means, the usual approach is to arrange a set of difference equations which approximate these differential equations over a set of finite mass elements. In such a system, then, derivatives become differences, and a solution is accomplished by the repetition of a prescribed series of numerical steps which solve the difference equations for new values of the parameters which would occur after a small time increment.

To formalize the differencing procedure, consider the transformation of the above differential equations to another set in which the independent variables are a dimensionless Lagrangean coordinate j and a dimensionless time n, and in which the masses are represented by integer values of j and the time by integer values of n.

The Jacobian for the Lagrangean coordinate system then follows from the differential equation representing conservation of mass.

$$\frac{\partial m(j)}{\partial j} = \frac{1}{3V(j,0)} \ \frac{\partial}{\partial j} \left[R(j,0) \right]^3 = \frac{1}{3V(j,n)} \ \frac{\partial}{\partial j} \left[R(j,n) \right]^3 . \quad (6)$$

The other conservation equations become

$$\left(\frac{\partial t}{\partial n}\right)^{-1} \frac{\partial u}{\partial n} = - R^2 \frac{\partial}{\partial j} (P + Q)\left(\frac{\partial m}{\partial j}\right)^{-1} \qquad \text{(momentum)}, \qquad (7)$$

$$\frac{\partial E}{\partial n} = - (P + Q) \frac{\partial V}{\partial n} + D \left(\frac{\partial t}{\partial n}\right) \qquad \text{(energy)}, \qquad (8)$$

and

$$u = \frac{\partial R}{\partial n} \left(\frac{\partial t}{\partial n}\right)^{-1} . \qquad (9)$$

In these equations the dependence of the variables on j and n has been
suppressed for simplicity.

The artificial viscosity may be variously defined, but the following
is a usual form:

$$Q = \frac{C}{V} \left(\frac{\partial u}{\partial j}\right)^2 \quad \text{if} \quad \frac{\partial u}{\partial j} < 0,$$

$$\qquad (10)$$

$$Q = 0 \qquad \text{if} \quad \frac{\partial u}{\partial j} \geqslant 0 ,$$

in which the value of C determines the amount of spreading of shocks.
When C is unity, the spread is about three zones, and when C is six the
spread is around six zones, the constant being proportional to the square
of the spread.[6,7]

In some unusual circumstances this form fails to provide the necessary
shock spreading. Such a case can arise in some problems involving imploding
shock waves.

A more rigorous form for the artificial viscosity, which is generally equivalent to the form above (Eq. (10)), is the following:

$$Q = \left(\frac{\partial m}{\partial j}\right)^2 \frac{C}{R^4 V} \left(\frac{\partial V}{\partial n}\right)^2 \left(\frac{\partial t}{\partial n}\right)^{-2} ,$$

$$\text{for } \frac{\partial V}{\partial n} < 0 ,$$

(11)

$$Q = 0 \text{ for } \frac{\partial V}{\partial n} \geq 0 .$$

The formation of a set of centered difference equations is now a matter of assigning integer values to the independent variables j and n and either defining the dependent variables at these points or at midpoints (at half integer points) in j or n. It is conventional to express the j and n values associated with a given parameter by subscripts and super-scripts, thus the radius at a mass point j and at a time t after n time increments $\Delta t(n) = \Delta t_n$ would appear as R_j^n.

The equations for the n-th time step $\Delta t^{n+\frac{1}{2}}$ over a set of mass elements $\Delta m_{j-\frac{1}{2}}$ follow.

$$u_j^{n+\frac{1}{2}} = u_j^{n-\frac{1}{2}} - \frac{\Delta t^n}{\Delta m_j} (R_j^n)^2 \left[P_{j+\frac{1}{2}}^n - P_{j-\frac{1}{2}}^n + Q_{j+\frac{1}{2}}^{n-\frac{1}{2}} - Q_{j-\frac{1}{2}}^{n-\frac{1}{2}} \right] , \qquad (12)$$

for which

$$\Delta m_j = \frac{1}{2} \Delta m_{j+\frac{1}{2}} + \frac{1}{2} \Delta m_{j-\frac{1}{2}}$$

and

$$\Delta t^n = \frac{1}{2} \Delta t^{n+\frac{1}{2}} + \frac{1}{2} \Delta t^{n-\frac{1}{2}} ,$$

$$R_j^{n+1} = R_j^n + u_j^{n+\frac{1}{2}} \Delta t^{n+\frac{1}{2}} , \qquad (13)$$
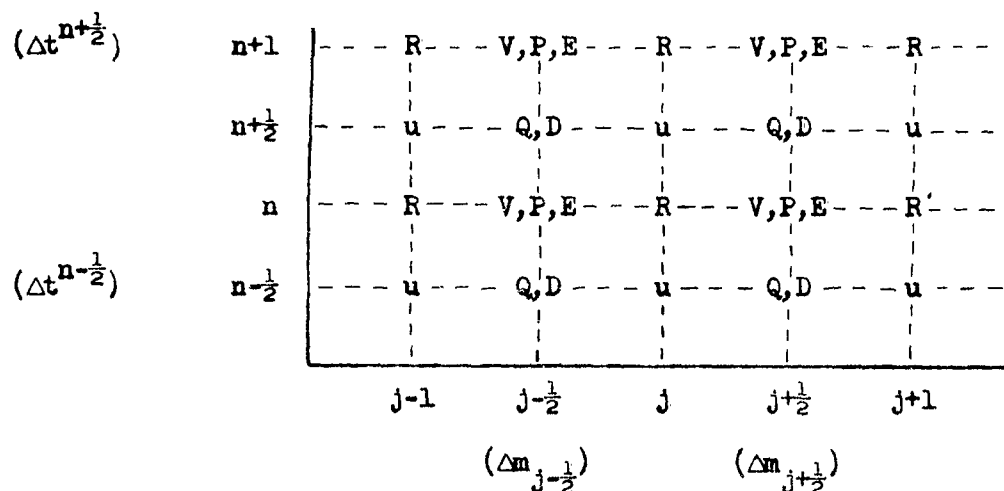
$$V_{j-\frac{1}{2}}^{n+1} = \frac{\left(R_j^{n+1} - R_{j-1}^{n+1}\right)}{3\Delta m_{j-\frac{1}{2}}} \left[\left(R_j^{n+1}\right)^2 + \left(R_j^{n+1}\right)\left(R_{j-1}^{n+1}\right) + \left(R_{j-1}^{n+1}\right)^2 \right], \qquad (14)$$

$$Q_{j-\frac{1}{2}}^{n+\frac{1}{2}} = C_1 \frac{\left[u_j^{n+\frac{1}{2}} - u_{j-1}^{n+\frac{1}{2}}\right]^2}{V_{j-\frac{1}{2}}^{n+1} + V_{j-\frac{1}{2}}^n} \quad \text{for} \quad u_j^{n+\frac{1}{2}} < u_{j-1}^{n+\frac{1}{2}}, \qquad (15)$$

$$Q_{j-\frac{1}{2}}^{n+\frac{1}{2}} = 0 \quad \text{for} \quad u_j^{n+\frac{1}{2}} > u_{j-1}^{n+\frac{1}{2}},$$

$$E_{j-\frac{1}{2}}^{n+1} = E_{j-\frac{1}{2}}^n - \left(\frac{1}{2} P_{j-\frac{1}{2}}^{n+1} + \frac{1}{2} P_{j-\frac{1}{2}}^n + Q_{j-\frac{1}{2}}^{n+\frac{1}{2}}\right)\left(V_{j-\frac{1}{2}}^{n+1} - V_{j-\frac{1}{2}}^n\right) + D_{j-\frac{1}{2}}^{n+\frac{1}{2}}. \qquad (16)$$

In these equations it is worth noting that the quantities are either
defined or averaged in such a way that first order errors in Δt or Δm
are avoided, i.e., the difference equations are centered. The actual
progression of the solution can better be illustrated by reference to a
space-time grid, as below, showing the points at which the various para-
meters are defined.

For illustration, assume that the n-th time step has been completed, and
that therefore all the values at times less than n are known, and that the

next step is to determine the values at $n+\frac{1}{2}$ and $n+1$ times. The difference equations have already been written down in the order in which they are computed. The first equation defines a new velocity at time $n+\frac{1}{2}$, at point j, in terms of the old velocity at that j-point at time $n-\frac{1}{2}$ and the radius at that j-point at time n, together with the pressure gradients at that point and at time n as represented by the differences in the pressures at j points $\frac{1}{2}$ a unit on either side of j. From this new velocity a new radius is computed in a straightforward manner, using the definition of the particle velocity. These new radii, in turn, are used to compute a new specific volume, and that new volume together with the new values of the velocity can be used to compute a new artificial viscosity. The artificial viscosity is nearly of second order in the time, and its lack of symmetry in the velocity equation does not disturb the degree of accuracy of these otherwise centered difference equations. The new volume, together with the new artificial viscosity, can then be used in the energy equation to determine a new energy and a new pressure. If the equation of state is not simple, it is then necessary to arrive at the new energy and pressure by some iterative method. The equation of state represents a second relation between these remaining two unknowns, i.e., the new energy and the new pressure. With a satisfactory solution for all of these parameters at a point j one can then advance to the next j-point and repeat the same procedure.

Of course, if the problem involves other mechanisms of energy transfer, or sources or sinks or energy, the term D in the energy equation becomes useful. If this term is to represent the diffusion of energy, either by radiation or by conduction, then the nature of the problem is changed, and

in most cases is made much more complicated. If for instance, radiation diffusion is to be considered, then the term D can be expressed as a gradient of a radiation energy flux.

$$D = - \left(\frac{\partial F}{\partial j}\right)\left(\frac{\partial m}{\partial j}\right)^{-1} ,$$

$$\text{(17)}$$

where

$$F = - \frac{acR^4}{3k} \left(\frac{\partial T^4}{\partial j}\right)\left(\frac{\partial m}{\partial j}\right)^{-1} ,$$

in which $k(T,V)$ represents a mean opacity, a is the radiation density constant and c is the speed of light. The inclusion of such terms however, couples the difference equations for energy conservation at each mass point, so that one then is faced with the solution of something like two-j simultaneous nonlinear equations, and the iterative procedure must become correspondingly more elegant.

The D term can also be used when a source of energy is required as an energy rate term or, when energy losses occur, as an energy sink. For instance, the D term can be used satisfactorily in detonation wave calculations. A number of forms to represent the burning of high explosives or gases in a detonation front are possible; one fairly crude but workable form is the following:

$$D_{j-\frac{1}{2}}^{n+1} = \frac{E_{Cj} \, \Delta t^{n+\frac{1}{2}}}{t_{Cj}} ,$$
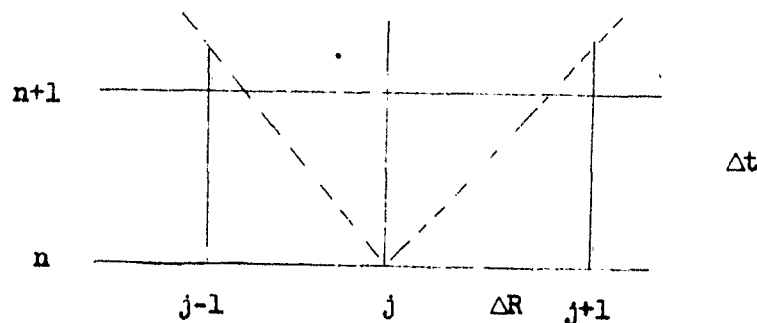
$$\text{(18)}$$

$$t_{Cj} = \frac{S \, \Delta R_{j-\frac{1}{2}}}{U_{Cj}} ,$$

in which E_{Cj} is the Chapman-Jouget energy, i.e., the energy generated in the detonation, U_{Cj} is the detonation velocity, and S is the spread or

thickness of the detonation front in keeping with the shock spreading characteristic of the artificial viscosity technique.

A great many cautions resulting from experience and from the details of the handling of the numerical procedure might well be included in a complete description of a numerical method, since many special considerations are necessary before a numerical program becomes truly workable. Some of these factors are concerned with the stability of the numerical procedure, attention to boundary conditions and initial conditions, techniques for expanding the grid system as shocks progress, and all the many problems of input and output, the storing of information, the stopping and restarting of the problem, and internal checks on the accuracy of the computation.

The stability criteria which must be considered are essential limitations on the size of the increments that can be permitted. The Courant Condition is a restriction on the time increment (Δt) such that local sounds or signals from one mass point will not have had time to reach beyond adjacent mass points in that length of time.

$$c < \frac{\Delta R}{\Delta t} \quad \text{or} \quad \Delta t < \frac{\Delta R}{c}$$

For an ideal gas $c = \gamma PV$ and generally $\Delta R \sim R^{-2} V \Delta m$, so that a sufficient condition for stability is

$$\Delta t^{n+\frac{1}{2}} < \left(\frac{V \Delta m}{R^2 \sqrt{\gamma PV}} \right)_{min} = \left(\frac{\Delta m}{R^2 \sqrt{\gamma P/V}} \right)_{min} \tag{19}$$

where γ is at least as large as the largest possible value of γ as determined by the equation of state. In shock fronts (or equivalently in compression regions) the artificial viscosity changes the nature of the differential equations from that of a wave equation to that of a diffusion-type equation, and another stability condition must be included on this account. An approximate derivation of this stability condition comes from the momentum equation in which

$$\frac{\partial u}{\partial t} \simeq - R^2 \frac{\partial}{\partial m} Q = - R^2 \frac{\partial}{\partial m} \left[\frac{C'}{V} \left(\frac{\partial u}{\partial m} \right)^2 \right] \;,$$

and from the conservation of mass,

$$V \sim R^2 \frac{\partial R}{\partial m} \quad \text{or} \quad \frac{1}{\Delta R} \sim \frac{R^2}{V} \frac{1}{\Delta m}$$

and

$$\frac{\Delta u}{\Delta t} \sim - \frac{C'}{\Delta R} \frac{(\Delta u)^2}{(\Delta m)^2}$$

or

$$\left(\frac{C' |\Delta u|}{\Delta R} \right) \frac{\Delta t}{(\Delta m)^2} \sim + 1 \quad (\text{for } \Delta u < 0)$$

for diffusion stability then, $\Delta t < \left(\frac{\Delta R}{C' |\Delta u|} \right) (\Delta m)^2$. Various approximate

forms of this inequality can be used, but perhaps the simplest results in

$$2C \frac{V_{j-\frac{1}{2}}^{n} - V_{j-\frac{1}{2}}^{n+1}}{V_{j-\frac{1}{2}}^{n+1}} < 1 \qquad (20)$$

where C is the constant in the artificial viscosity (Eq. (10)).

The boundary conditions at the origin in cylindrical or spherical geometries are particularly easily satisfied with the numerical scheme dealt with here, since it is only necessary to note that the velocity and radius is initially zero at the origin and then to avoid changing them in the computation loops by always starting a cycle with the compute of the velocity and radius at the first point away from the origin. The artificial viscosity removes the necessity of any complications with floating boundary conditions such as a shock front might otherwise present, and the other boundary conditions in a Lagrangean system are most often straightforwardly expressed from the physical restraints of the problem. For instance, if the calculation is of an explosion in air, the boundary condition at the front of the explosion may easily be the conditions of the ambient air in undisturbed zones ahead of any shock. When the last zone is about to be influenced by the shock, e.g., its temperature or velocity are about to rise, then another undisturbed zone can be added if it is desirable to keep a limited number of mass zones in the problem, then a scheme can be arranged whereby when a zone is added some other pair of zones is combined into one zone, keeping the number of zones fixed. Care should be taken in such an exercise to observe the usual conservations of mass, momentum and energy by altering the velocities and internal energies of the resulting combined zone accordingly.

Stating boundary conditions for moving pistons or for free surfaces
blowing off into a vacuum involves no more serious complication to the
code than to alter the details of how each cycle is begun or ended. For
example in the blow-off situation each cycle is stopped at the last zone,
regardless of its velocity or temperature. For piston motion, on the other
hand, a separate prescription must be provided for the piston velocity or
its position, but then the usual equations are followed for each mass
point $R_0^n = f(t$ or $n)$, $u_0^n = g(t$ or $n)$. The specification of initial
conditions (or boundary conditions, for that matter) is a matter of
stating the physics of a problem in terms of initial values of a set of
representative variables such as the velocities, temperatures and densities
of all the mass elements at some instant of time.

Shells or layers of different materials, having different densities
and thermodynamic properties can be most easily managed on a Lagrangean
system, since keeping the materials separate and treating each differently
only involves using different equations of state according to which j-
values (mass elements) the computation is working on.

Numerical techniques of the form described here possess such
generality that results may include quite unexpected features such as
unpredicted shocks. So much freedom or lack of forcing in the form or
nature of solutions makes the method at once very powerful and yet injects
more of an experimental physics flavor into the procedure in contrast to
the physical clarity of analytic results. For this very reason, the
processing and ultimate analysis of numerical results is a vital part of
this approach to problem solving in physics.

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